



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2024 – 07:37 AM EDT

PDB ID : 4YLO
Title : E. coli Transcription Initiation Complex - 16-bp spacer and 4-nt RNA
Authors : Zuo, Y.; Steitz, T.A.
Deposited on : 2015-03-05
Resolution : 6.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

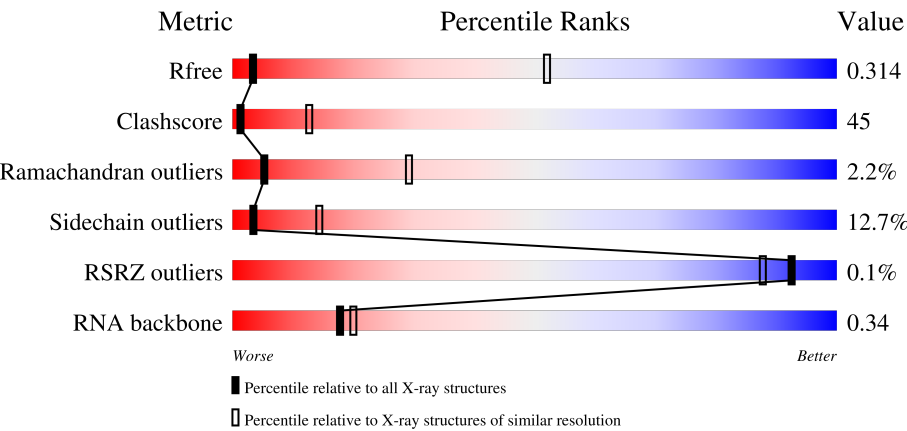
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1083 (8.00-4.00)
Clashscore	180529	1124 (8.00-4.00)
Ramachandran outliers	177936	1015 (8.00-3.98)
Sidechain outliers	177891	1019 (8.00-3.96)
RSRZ outliers	164620	1078 (8.00-4.00)
RNA backbone	3690	1173 (8.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	242	<div><div></div><div>47%40%8%5%</div></div>
1	B	242	<div><div></div><div>41%47%6%6%</div></div>
1	G	242	<div><div></div><div>41%48%7%5%</div></div>
1	H	242	<div><div></div><div>45%44%5%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	M	242	
1	N	242	
2	C	1342	
2	I	1342	
2	O	1342	
3	D	1407	
3	J	1407	
3	P	1407	
4	E	90	
4	K	90	
4	Q	90	
5	F	628	
5	L	628	
5	R	628	
6	1	49	
6	4	49	
6	7	49	
7	2	49	
7	5	49	
7	8	49	
8	3	4	
8	6	4	
8	9	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	D	1502	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 94608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	B	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	G	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	H	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			
1	M	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	N	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP A7ZSI4
A	-5	HIS	-	expression tag	UNP A7ZSI4
A	-4	HIS	-	expression tag	UNP A7ZSI4
A	-3	HIS	-	expression tag	UNP A7ZSI4
A	-2	HIS	-	expression tag	UNP A7ZSI4
A	-1	HIS	-	expression tag	UNP A7ZSI4
A	0	HIS	-	expression tag	UNP A7ZSI4
B	-6	ALA	-	expression tag	UNP A7ZSI4
B	-5	HIS	-	expression tag	UNP A7ZSI4
B	-4	HIS	-	expression tag	UNP A7ZSI4
B	-3	HIS	-	expression tag	UNP A7ZSI4
B	-2	HIS	-	expression tag	UNP A7ZSI4
B	-1	HIS	-	expression tag	UNP A7ZSI4
B	0	HIS	-	expression tag	UNP A7ZSI4
G	-6	ALA	-	expression tag	UNP A7ZSI4
G	-5	HIS	-	expression tag	UNP A7ZSI4
G	-4	HIS	-	expression tag	UNP A7ZSI4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	HIS	-	expression tag	UNP A7ZSI4
G	-2	HIS	-	expression tag	UNP A7ZSI4
G	-1	HIS	-	expression tag	UNP A7ZSI4
G	0	HIS	-	expression tag	UNP A7ZSI4
H	-6	ALA	-	expression tag	UNP A7ZSI4
H	-5	HIS	-	expression tag	UNP A7ZSI4
H	-4	HIS	-	expression tag	UNP A7ZSI4
H	-3	HIS	-	expression tag	UNP A7ZSI4
H	-2	HIS	-	expression tag	UNP A7ZSI4
H	-1	HIS	-	expression tag	UNP A7ZSI4
H	0	HIS	-	expression tag	UNP A7ZSI4
M	-6	ALA	-	expression tag	UNP A7ZSI4
M	-5	HIS	-	expression tag	UNP A7ZSI4
M	-4	HIS	-	expression tag	UNP A7ZSI4
M	-3	HIS	-	expression tag	UNP A7ZSI4
M	-2	HIS	-	expression tag	UNP A7ZSI4
M	-1	HIS	-	expression tag	UNP A7ZSI4
M	0	HIS	-	expression tag	UNP A7ZSI4
N	-6	ALA	-	expression tag	UNP A7ZSI4
N	-5	HIS	-	expression tag	UNP A7ZSI4
N	-4	HIS	-	expression tag	UNP A7ZSI4
N	-3	HIS	-	expression tag	UNP A7ZSI4
N	-2	HIS	-	expression tag	UNP A7ZSI4
N	-1	HIS	-	expression tag	UNP A7ZSI4
N	0	HIS	-	expression tag	UNP A7ZSI4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	I	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			
2	O	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			
3	P	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	Q	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	L	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			
5	R	497	Total	C	N	O	S	0	0	0
			4022	2512	719	768	23			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	THR	-	expression tag	UNP P00579
L	-14	MET	-	expression tag	UNP P00579
L	-13	ARG	-	expression tag	UNP P00579
L	-12	GLY	-	expression tag	UNP P00579
L	-11	SER	-	expression tag	UNP P00579
L	-10	HIS	-	expression tag	UNP P00579
L	-9	HIS	-	expression tag	UNP P00579
L	-8	HIS	-	expression tag	UNP P00579
L	-7	HIS	-	expression tag	UNP P00579
L	-6	HIS	-	expression tag	UNP P00579
L	-5	HIS	-	expression tag	UNP P00579
L	-4	THR	-	expression tag	UNP P00579
L	-3	ASP	-	expression tag	UNP P00579
L	-2	GLN	-	expression tag	UNP P00579
L	-1	PHE	-	expression tag	UNP P00579
L	0	THR	-	expression tag	UNP P00579
R	-14	MET	-	expression tag	UNP P00579
R	-13	ARG	-	expression tag	UNP P00579
R	-12	GLY	-	expression tag	UNP P00579
R	-11	SER	-	expression tag	UNP P00579
R	-10	HIS	-	expression tag	UNP P00579
R	-9	HIS	-	expression tag	UNP P00579
R	-8	HIS	-	expression tag	UNP P00579
R	-7	HIS	-	expression tag	UNP P00579
R	-6	HIS	-	expression tag	UNP P00579
R	-5	HIS	-	expression tag	UNP P00579
R	-4	THR	-	expression tag	UNP P00579
R	-3	ASP	-	expression tag	UNP P00579
R	-2	GLN	-	expression tag	UNP P00579
R	-1	PHE	-	expression tag	UNP P00579
R	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a DNA chain called NT strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	4	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			
6	7	49	Total	C	N	O	P	0	0	0
			996	476	178	294	48			

- Molecule 7 is a DNA chain called T strand DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	5	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			
7	8	49	Total	C	N	O	P	0	0	0
			1012	481	191	292	48			

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*AP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	6	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			
8	9	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Mg	0	0
			1	1		
9	J	1	Total	Mg	0	0
			1	1		
9	P	1	Total	Mg	0	0
			1	1		

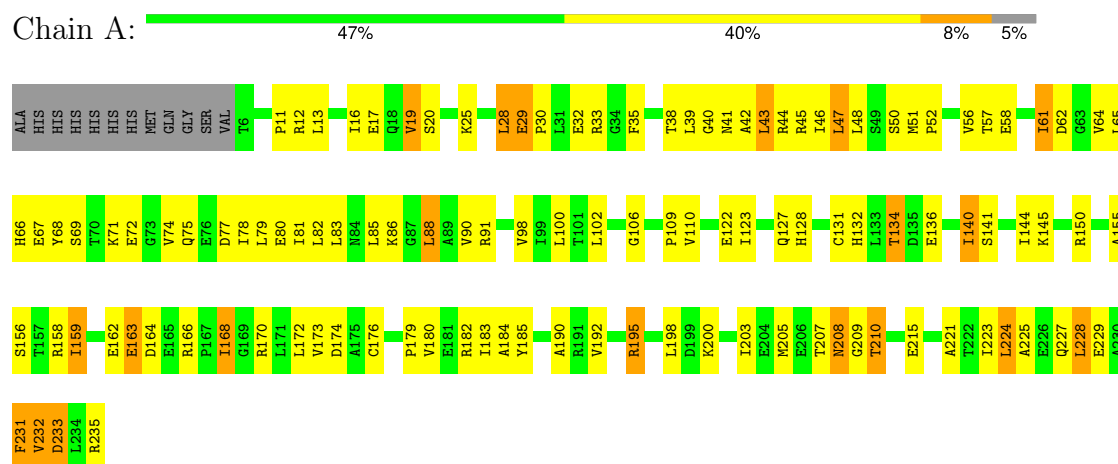
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		
10	J	2	Total	Zn	0	0
			2	2		
10	P	2	Total	Zn	0	0
			2	2		

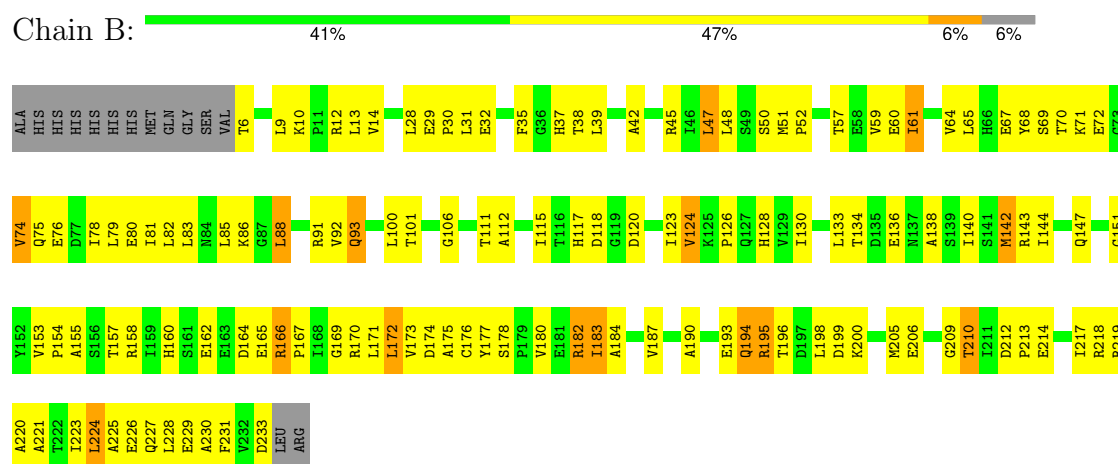
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

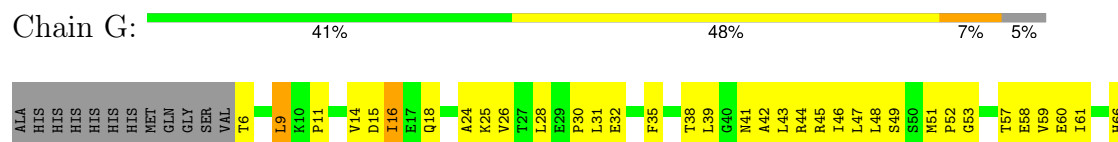
• Molecule 1: DNA-directed RNA polymerase subunit alpha

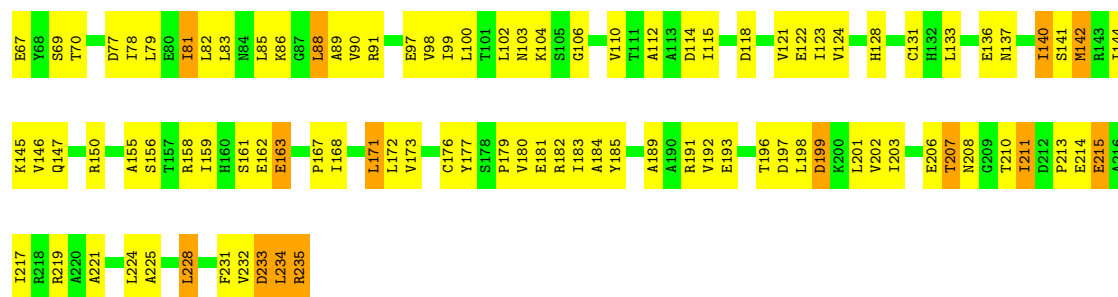


• Molecule 1: DNA-directed RNA polymerase subunit alpha



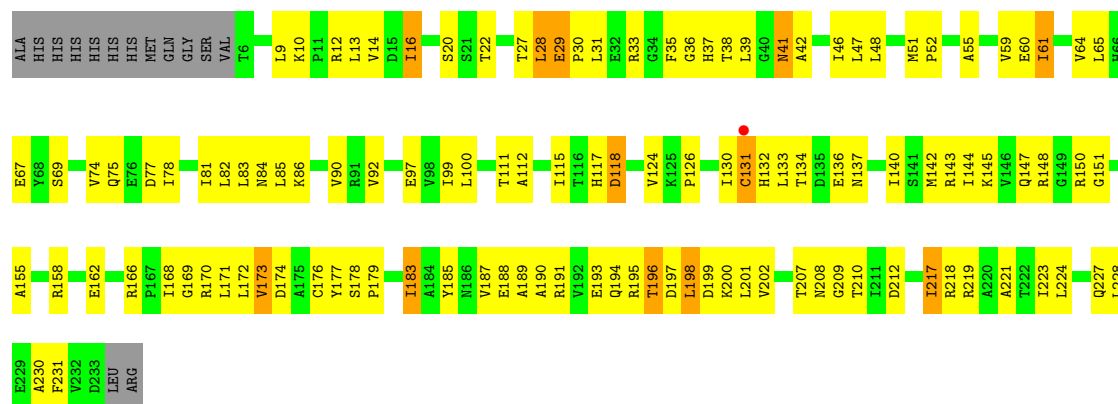
• Molecule 1: DNA-directed RNA polymerase subunit alpha





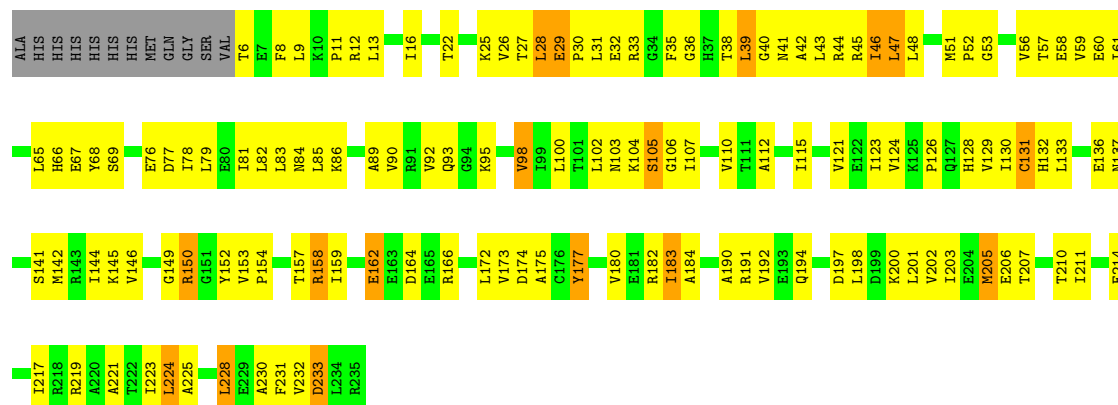
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain H: 45% 44% 5% 6%



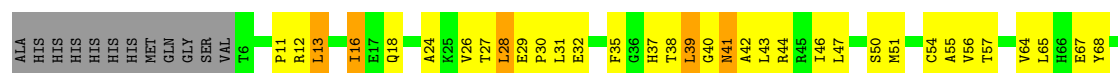
• Molecule 1: DNA-directed RNA polymerase subunit alpha

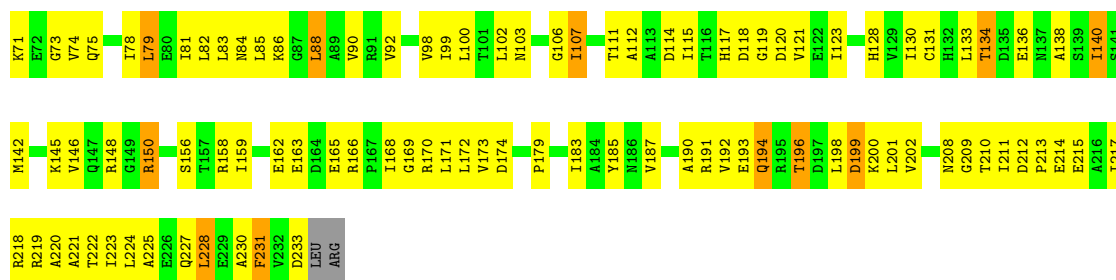
Chain M: 40% 48% 7% 5%



• Molecule 1: DNA-directed RNA polymerase subunit alpha

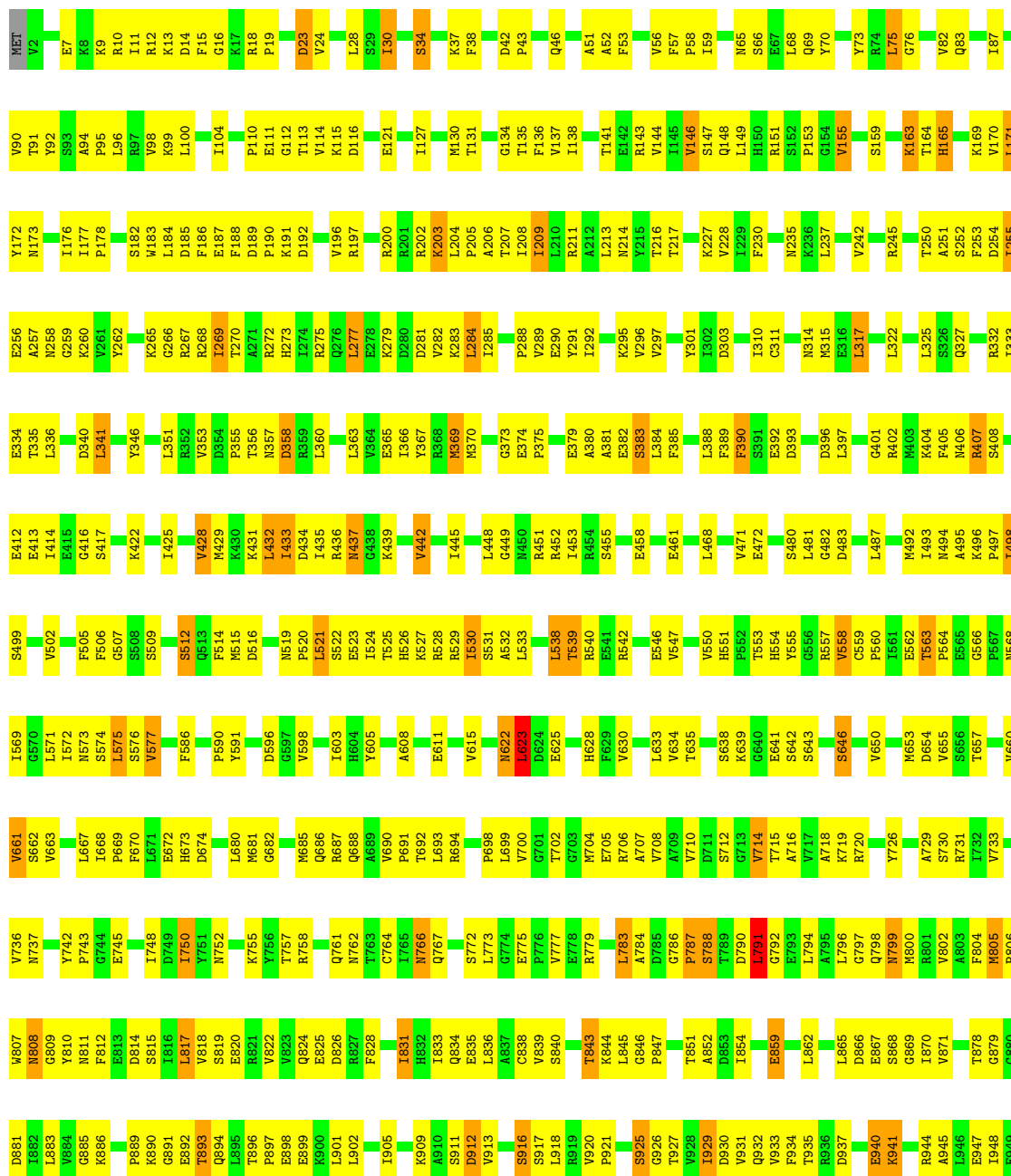
Chain N: 40% 47% 7% 6%





• Molecule 2: DNA-directed RNA polymerase subunit beta

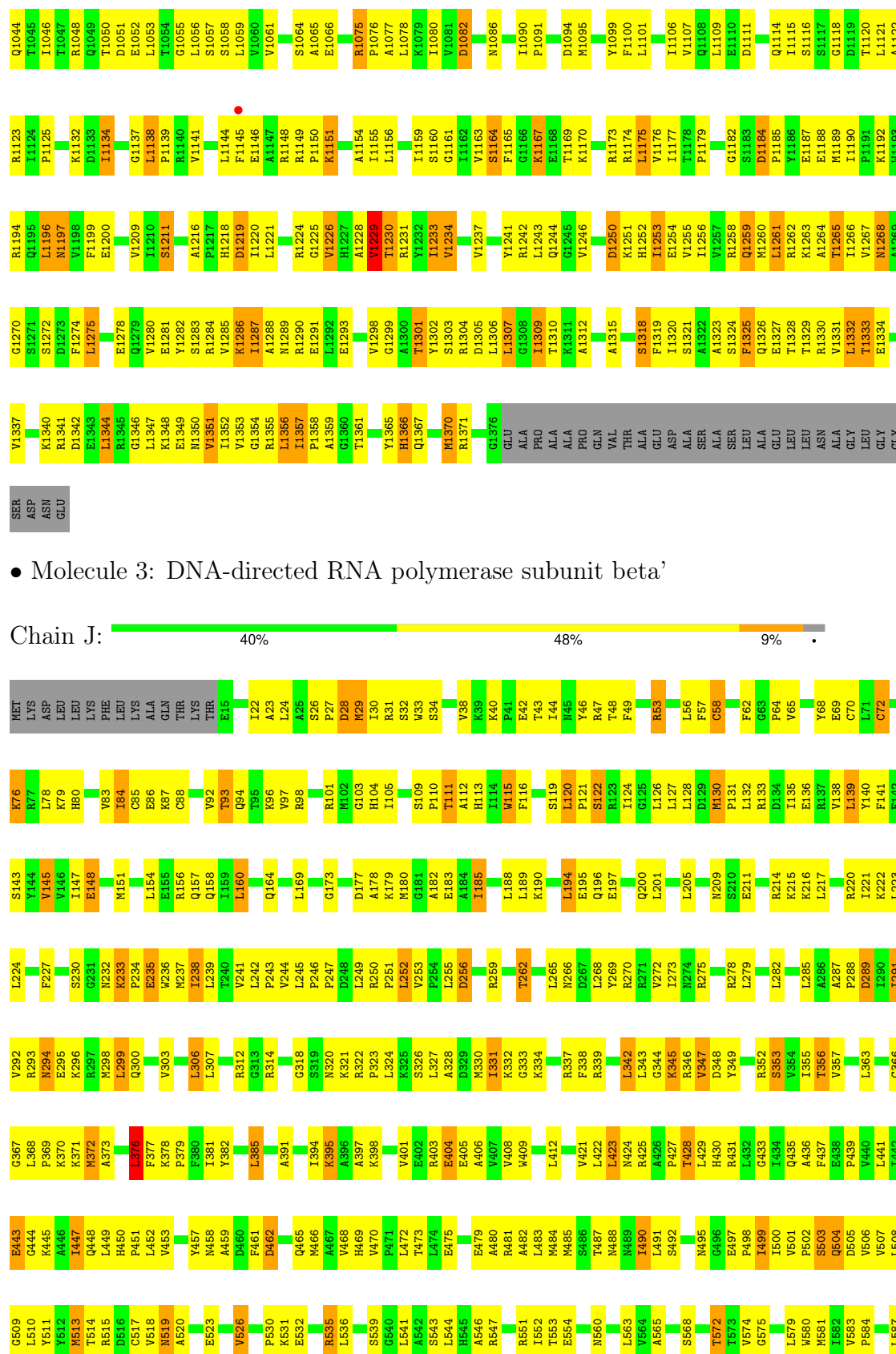
Chain C: 45% 48% 6%

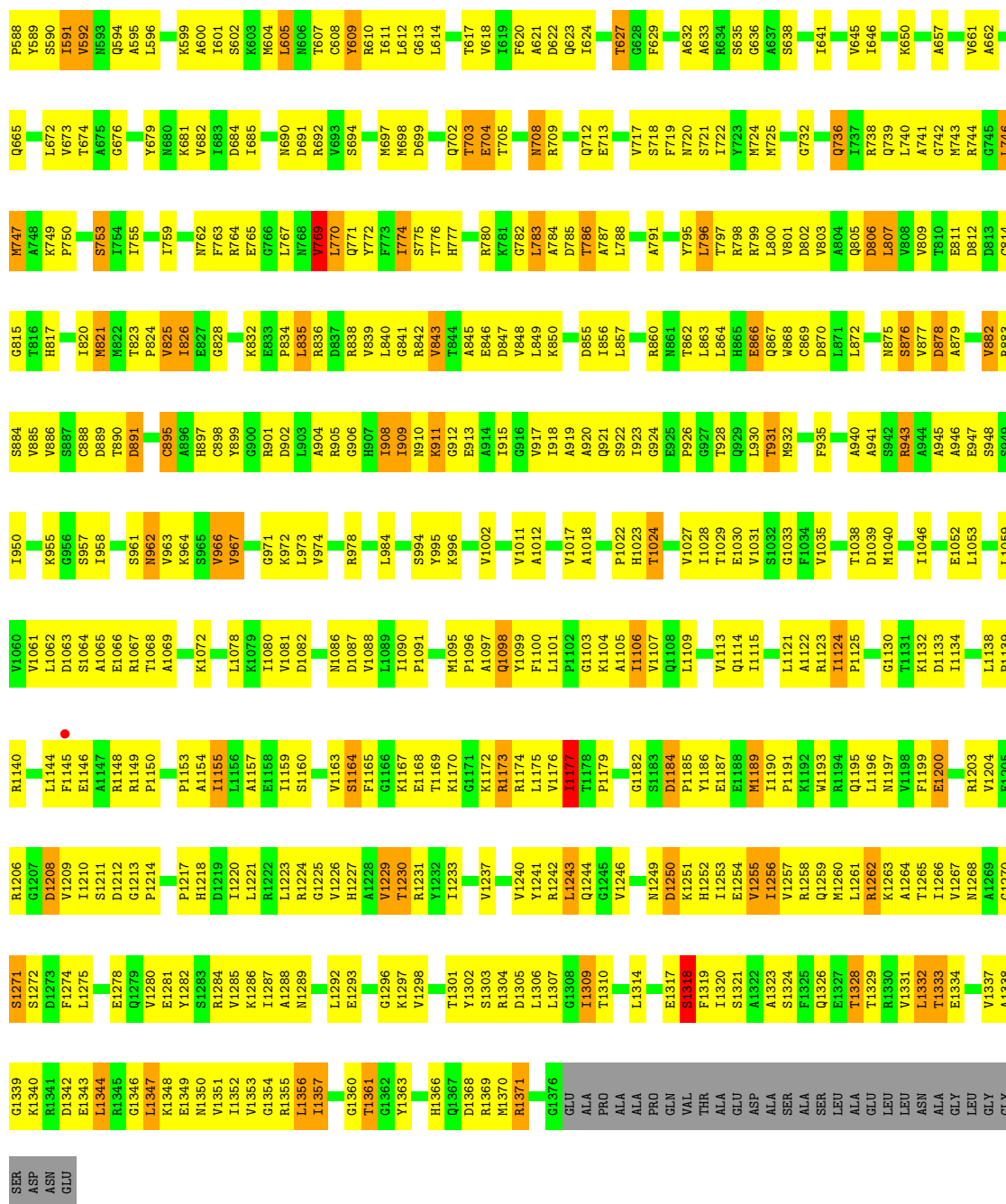


- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:  36% 51% 10%

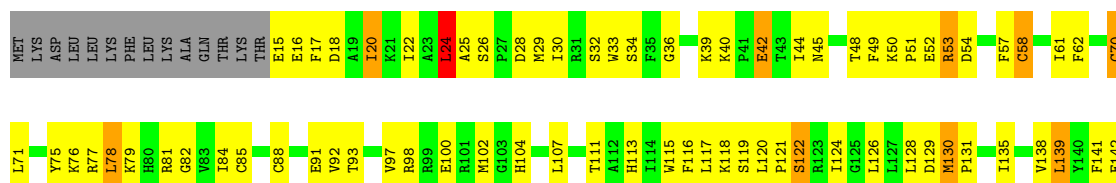
MET	V65	L132	N206	R270	R339	V407	A476	S543	T617	R692	P758	I826	T890	G969
LYS	K66	R133	E207	R271	Q340	V408	Q477	L544	V618	R693	I759	E827	D891	S969
ASP	D67	D134	T208	V272	N341	N409	L478	HE45	T619	V693	I760	G829	G892	S970
LEU	V68	T135	N209	R275	L342	D410	E479	A546	F620	G694	T760	G829	G893	G971
LEU	E69	E136	E210	R276	L343	D413	A480	RE47	A621	K695	A761	D830	V894	L973
LYS	C70	R137	E211	N276	G344	D413	A481	V548	D622	A696	N762	D831	C895	L973
PHE	L71	V138	T212	N277	K345	D413	A482	R551	Q623	M697	T763	K832	A896	V974
LEU	K74	L139	K213	R278	R346	T416	L483	R552	I624	N700	R764	E833	H897	T975
LYS	K75	Y140	K214	L279	V347	R417	L484	I552	M625	T701	E765	P834	C898	T976
ALA	K76	F141	K215	K280	D348	E418	M485	V555	Y626	Q702	G766	R835	G900	S977
GLN	R77	E142	K215	R281	V349	H419	S486	T555	T627	T703	L767	R836	G900	S977
THR	R78	E145	T218	L282	S350	P420	T487	D558	G628	E704	N768	D837	R901	T979
LYS	K79	V146	K219	L283	G351	V421	M488	A559	F629	E705	T769	R838	D902	T980
THR	R80	V147	K220	D284	R352	L422	M489	N560	A632	T706	L770	V839	L903	E981
E15	H81	I147	K221	L285	V353	L423	L490	N560	A632	V706	Q771	L840	A904	
E16	R80	M151	K222	L285	N354	L424	L491	L563	S635	I707	Y772	G841		L984
F17	H81	M151	L223	D289	T355	N424	L491	L563	S635	R708	Y772	R842		L985
D18	V83	E155	L224	I290	T356	A426	S492	L563	S635	R709	I774	V843		L986
A19	L84	R156	E225	D293	V357	P427	M495	T572	A637	D710	S775	T844		
L20	V90	E159	K226	R293	G358	T428	G496	T573	S638	G711		A845		
K21	E91	T159	F227	K296	P359	L429	E497	V574	V639	Q712	A779	E846		
A23	V92	L160	Q228	R297	R362	H430	P498	G575	G640	E713	R780	D847		
L24	T93	T161	S230	K298	L363	R431	P499	R576	I641	E714	K781	V848		
A25	Q94	E162	S231	L298	L363	L432	V501	A577	D642	K715	G782	L849		
S26	T95	E183	N232	Q300	G366	T434	P502	L579	M644	K716	L783	K850		
P27	A96	Q164	K233	E301	G367	Q435	S503		V645	S718	T786	T853		
D28	V97	Q164	P234	V303	L368	A436	Q504	V583	I646	F719	A787	A854		
M29	R98	L169	E235	V303	P369	F437	D505	P584	P647	N720	L788	D855		
R31	R99	G173	W236	L306	K370	E438	V506	K685		S721		I856		
S32	E100	D174	W237	L307	K371	P439	V507	G586	K650	I722	Y795	L857		
W33	R101	E175	T238	L308	K372	V440	L508	L587	H651	I723	L796	V858		
S34	H104	A178	L242	D308	A373	L441	G509	S590	I654	M724	T797	P859		
F35	I105	E106	P243	R312	E375	L442	L510	S590	I654	M725	R798	R860		
C36	L107	E107	V244	G313	L376	T442	L510	S590	I654	M726	R799	T861		
E37	A108	A108	L245	G313	F377	E443	N513	V592	A657	S727	L800	T862		
K40	S109	S109	P246	T316	R379	E443	N513	V592	A657	S728	L801	L863		
P41	T110	T111	P247	T317	F380	H450	V518	Q594	E658	R731	D802	L864		
E42	A112	Q186	D248	G318	F380	H450	V518	Q594	E658	Q732	V803	C869		
T43	H113	A187	L249	S319	L381	L452	N519	A595	E660	S733	Q805	D870		
I44	T114	A187	R250	G383	Y382	V453	A520	L596	A662	A734	D806	L871		
R47	W115	L188	P251	K321	G383	V457	K521	K599	E663	A735	L807	L872		
T48	F116	L189	L252	R322	K384	Y457	G522	A600	I664	T736	V808	E873		
F49	L117	K190	P254	R322	L385	Y457	G522	A600	Q665	I737	V809	E874		
R53	L120	D193	L255	K325	L387	F461	G524	S602	F668	T810	T810	N875		
D54	P121	D194	R259	S326	L387	D462	G524	S602	F668	Q739	E811	S876		
S55	S122	E195	F260	K326	A391	D464	V526	M604	L672	A741	D813	V877		
L56	R123	Q196	T260	D329	K395	M466	V526	M604	L672	A741	D813	V877		
F57	I124	E197	T262	K330	A396	A467	P530	Q508	T674	Q745	G819	R882		
C58	G125	C198	S263	L331	A397	H469	K531	Y609	R678	L746	G819	R883		
A59	L126	G125	D264	K332	A398	V470	E532	R610	V679	M747	R820	S884		
R60	L127	L201	D265	G333	K398	P471	L536	L611	N680	A748	W821	V885		
L61	L128	R202	V266	K334	V401	L472	L536	G613	K681	K749	W822	V886		
F62	D129	E203	D267	K337	E404	T473	V537	L615	V682	P750	T823	S987		
G63	M130	E204	L268	R337	E404	L474	V537	L615	V682	P750	T823	S987		
P64	L205	L205	V269	F338	E404	E475	A542	P616	D684	I755	V825	D889		





• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain P: 40% 48% 8%

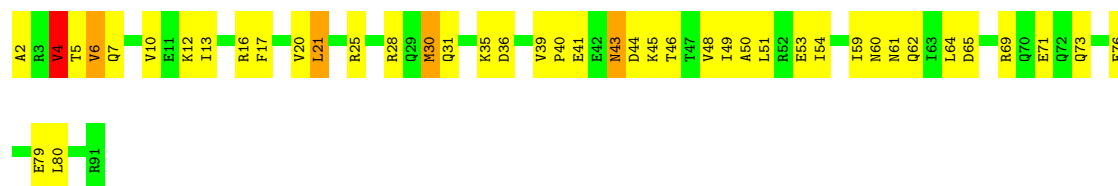


D1184	K1104	V1027	A944	Q867	S793	S723	D643	I578	Y512	I442	L374	R312	L223	V146
P1186	L1109	I1028	E947	Q868	G794	I722	D644	L579	R513	E443	E376	G313	F227	I147
Y1186	Y936	T1029	S948	C969	Y795	Y723	V645	W580	T514	Q448	L376	A315	E148	E148
E1187	V1113	E1030	S949	C969	Y796	Y724	V646	W581	R515	Q449	F377	A316	K233	T152
E1188	G1114	S1031	I950	E873	L797	Y725	I646	I582	D516	L449	K378	T317	K234	T152
M1189	I1115	S1032	Q951	E874	R798	S728	E648	P584	V518	H450	P379	G318	E285	E155
I1190	V1035	V1035	Q952	E875	R799	S728	E649	K585	R519	L452	I381	S319	W236	E155
I1191	R1036	R1036	S876	R876	L800	R731	K650	G586	A520	V453	Y382	K321	W237	Q158
K1192	F1037	F1037	S877	R877	V801	R731	K651	L587	E521	Y457	G383	K322	T238	I159
W1193	T1038	T1038	D878	V878	D802	A734	I654	P588	E523	D462	L324	P323	L239	L160
R1194	A1122	A1122	K959	K959	V803	A735	I655	S590	R524	D463	L325	K325	L242	T161
Q1195	L1130	L1130	K881	V882	R804	Q736	A657	S590	R525	Q463	A391	K326	P243	E162
L1196	T1131	T1131	V883	D806	Q805	I737	E658	I591	V526	Q464	T392	S326	V244	E163
F1199	K1132	K1132	S884	L807	R806	Q738	V661	V592	T528	Q465	T393	L327	V245	Q164
E1200	I1046	I1046	V885	V885	L740	Q739	I661	N593	G529	M466	I394	A328	P246	Y165
	T1047	T1047	T930	V894	V808	L740	I664	M604	P529	A467	A397	D329	P247	L166
			T931	V895	G815	A741	I665	L605	K531	V468	K388	M330	D248	L169
			T816	T816	T810	G742	Q665	K599	E532	H469	K389	I331	L249	
			T820	T820	E811	R743	F668	A600	E533	V470	K390	K332	R250	
			T821	T821	D812	R744	I668	I601	E534	L472	M400	G333	P251	G173
			T822	T822	C814	G745	I669	L612	R535	L473	V401	K334	L252	D174
			T823	T823	D815	L746	I670	M603	L536	T473	E402	Q335	V253	E175
			T824	T824	G816	I671	I671	L606	Y537	L474	R403	G336	P254	E176
			T825	T825	T817	I672	I672	L607	R538	E475	E404	R337	L255	D177
			T826	T826	T818	I673	I673	L608		A476	A405	F338	D256	A178
			T827	T827	T819	I674	I674	L609		Q477	A406	K179		K179
			T828	T828	T820	I675	I675	L610		E478	V407	R259		M180
			T829	T829	T821	I676	I676	L611		E479	V408	Q341		G181
			T830	T830	T822	I677	I677	L612		A480	I411	L342	A261	A182
			T831	T831	T823	I678	I678	L613		A481	L412	L343	T262	
			T832	T832	T824	I679	I679	L614		A482	V415	G344	S263	I185
			T833	T833	T825	I680	I680	L615		A483	I416	K345	D264	L188
			T834	T834	T826	I681	I681	L616		A484	I417	R346	L265	L189
			T835	T835	T827	I682	I682	L617		A485	E418	V347	L268	
			T836	T836	T828	I683	I683	L618		A486	R417	D348	Y269	
			T837	T837	T829	I684	I684	L619		A487	E419	Y349	R270	M192
			T838	T838	T830	I685	I685	L620		A488	P420	G351	R271	E195
			T839	T839	T831	I686	I686	L621		A489	V421	R352	V272	E195
			T840	T840	T832	I687	I687	L622		A490	L422	S353	I273	L201
			T841	T841	T833	I688	I688	L623		A491	L423	V354	I274	L201
			T842	T842	T834	I689	I689	L624		A492	M424	I355	R275	L205
			T843	T843	T835	I690	I690	L625		A493	R425	T356	R278	
			T844	T844	T836	I691	I691	L626		A494	A426	R362	L285	T208
			T845	T845	T837	I692	I692	L627		A495	P427	L363	E211	N209
			T846	T846	T838	I693	I693	L628		A496	I428	R364	T212	S210
			T847	T847	T839	I694	I694	L629		A497	E429	L365	K213	E211
			T848	T848	T840	I695	I695	L630		A498	P498	Q366	R214	K215
			T849	T849	T841	I696	I696	L631		A499	I500	C367	L298	K216
			T850	T850	T842	I697	I697	L632		A500	R431	L368	L299	L217
			T851	T851	T843	I698	I698	L633		A501	L432	D505	V303	T218
			T852	T852	T844	I699	I699	L634		A502	R432	P369	L306	K219
			T853	T853	T845	I700	I700	L635		A503	L433	K370	L307	K219
			T854	T854	T846	I701	I701	L636		A504	R433	R371	L308	R220
			T855	T855	T847	I702	I702	L637		A505	E434	K372	L309	I221
			T856	T856	T848	I703	I703	L638		A506	P437	L373	L310	K222
			T857	T857	T849	I704	I704	L639		A507	E438	K374	L311	
			T858	T858	T850	I705	I705	L640		A508	P439	K375	L312	
			T859	T859	T851	I706	I706	L641		A509	V440	K376	L313	
			T860	T860	T852	I707	I707	L642		A510	E441	K377	L314	
			T861	T861	T853	I708	I708	L643		A511	P442	K378	L315	
			T862	T862	T854	I709	I709	L644		A512	E442	K379	L316	
			T863	T863	T855	I710	I710	L645		A513	P443	K380	L317	
			T864	T864	T856	I711	I711	L646		A514	E443	K381	L318	
			T865	T865	T857	I712	I712	L647		A515	P444	K382	L319	
			T866	T866	T858	I713	I713	L648		A516	E444	K383	L320	
			T867	T867	T859	I714	I714	L649		A517	P445	K384	L321	
			T868	T868	T860	I715	I715	L650		A518	E445	K385	L322	
			T869	T869	T861	I716	I716	L651		A519	P446	K386	L323	
			T870	T870	T862	I717	I717	L652		A520	E446	K387	L324	
			T871	T871	T863	I718	I718	L653		A521	P447	K388	L325	
			T872	T872	T864	I719	I719	L654		A522	E447	K389	L326	
			T873	T873	T865	I720	I720	L655		A523	P448	K390	L327	
			T874	T874	T866	I721	I721	L656		A524	E448	K391	L328	
			T875	T875	T867	I722	I722	L657		A525	P449	K392	L329	
			T876	T876	T868	I723	I723	L658		A526	E449	K393	L330	
			T877	T877	T869	I724	I724	L659		A527	P450	K394	L331	
			T878	T878	T870	I725	I725	L660		A528	E450	K395	L332	
			T879	T879	T871	I726	I726	L661		A529	P451	K396	L333	
			T880	T880	T872	I727	I727	L662		A530	E451	K397	L334	
			T881	T881	T873	I728	I728	L663		A531	P452	K398	L335	
			T882	T882	T874	I729	I729	L664		A532	E452	K399	L336	
			T883	T883	T875	I730	I730	L665		A533	P453	K400	L337	
			T884	T884	T876	I731	I731	L666		A534	E453	K401	L338	
			T885	T885	T877	I732	I732	L667		A535	P454	K402	L339	
			T886	T886	T878	I733	I733	L668		A536	E454	K403	L340	
			T887	T887	T879	I734	I734	L669		A537	P455	K404	L341	
			T888	T888	T880	I735	I735	L670		A538	E455	K405	L342	
			T889	T889	T881	I736	I736	L671		A539	P456	K406	L343	
			T890	T890	T882	I737	I737	L672		A540	E456	K407	L344	
			T891	T891	T883	I738	I738	L673		A541	P457	K408	L345	
			T892	T892	T884	I739	I739	L674		A542	E457	K409	L346	
			T893	T893	T885	I740	I740	L675		A543	P458	K410	L347	
			T894	T894	T886	I741	I741	L676		A544	E458	K411	L348	
			T895	T895	T887	I742	I742	L677		A545	P459	K412	L349	
			T896	T896	T888	I743	I743	L678		A546	E459	K413	L350	
			T897	T897	T889	I744	I744	L679		A547	P460	K414	L351	
			T898	T898	T890	I745	I745	L680		A548	E460	K415	L352	
			T899	T899	T891	I746	I746	L681		A549	P461	K416	L353	
			T900	T900	T892	I747	I747	L682		A550	E461	K417	L354	
			T901	T901	T893	I748	I748	L683		A551	P462	K418	L355	
			T902	T902	T894	I749	I749	L684		A552	E462	K419	L356	
			T903	T903	T895	I750	I750	L685		A553	P463	K420	L357	
			T904	T904	T896	I751	I751	L686		A554	E463	K421	L358	
			T905	T905	T897	I752	I752	L687		A555	P464	K422	L359	
			T906	T906	T898	I753	I753	L688		A556	E464	K423	L360	
			T907	T907	T899	I754	I754	L689		A557	P465	K424	L361	
			T908	T908	T900	I755	I755	L690		A558	E465	K425	L362	
			T909	T909	T901	I756	I756	L691		A559	P466	K426	L363	
			T910	T910	T902	I757	I757	L692		A560	E466	K427	L364	
			T911	T911	T903	I758	I758	L693		A561	P467	K428	L365	
			T912	T912	T904</									



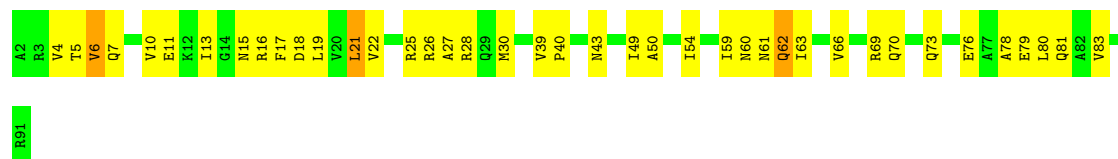
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 52% 42%



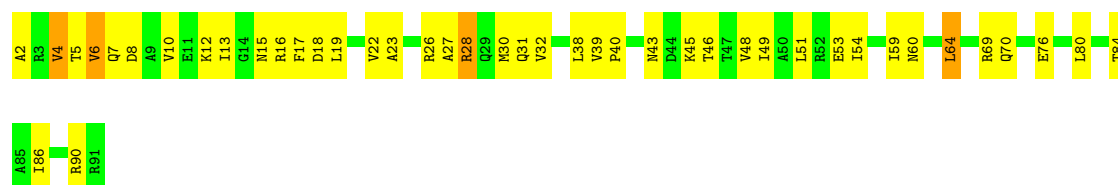
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 56% 41%



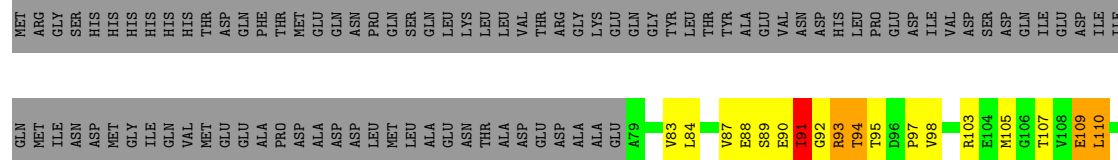
- Molecule 4: DNA-directed RNA polymerase subunit omega

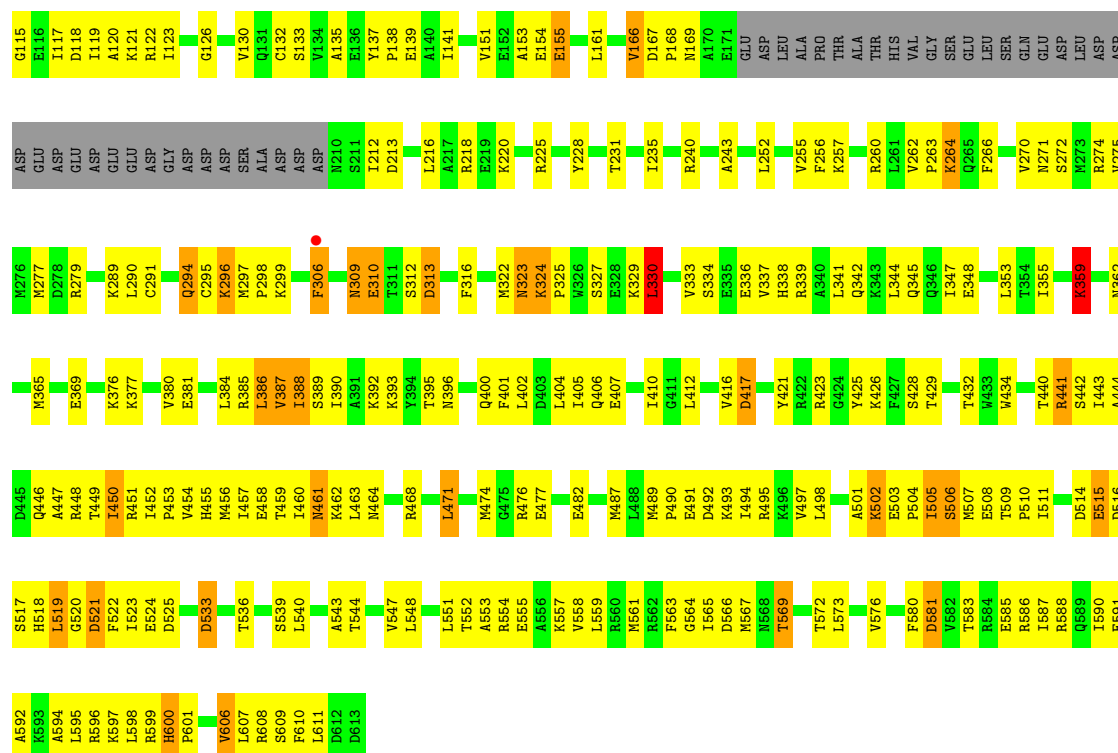
Chain Q: 52% 43%



- Molecule 5: RNA polymerase sigma factor RpoD

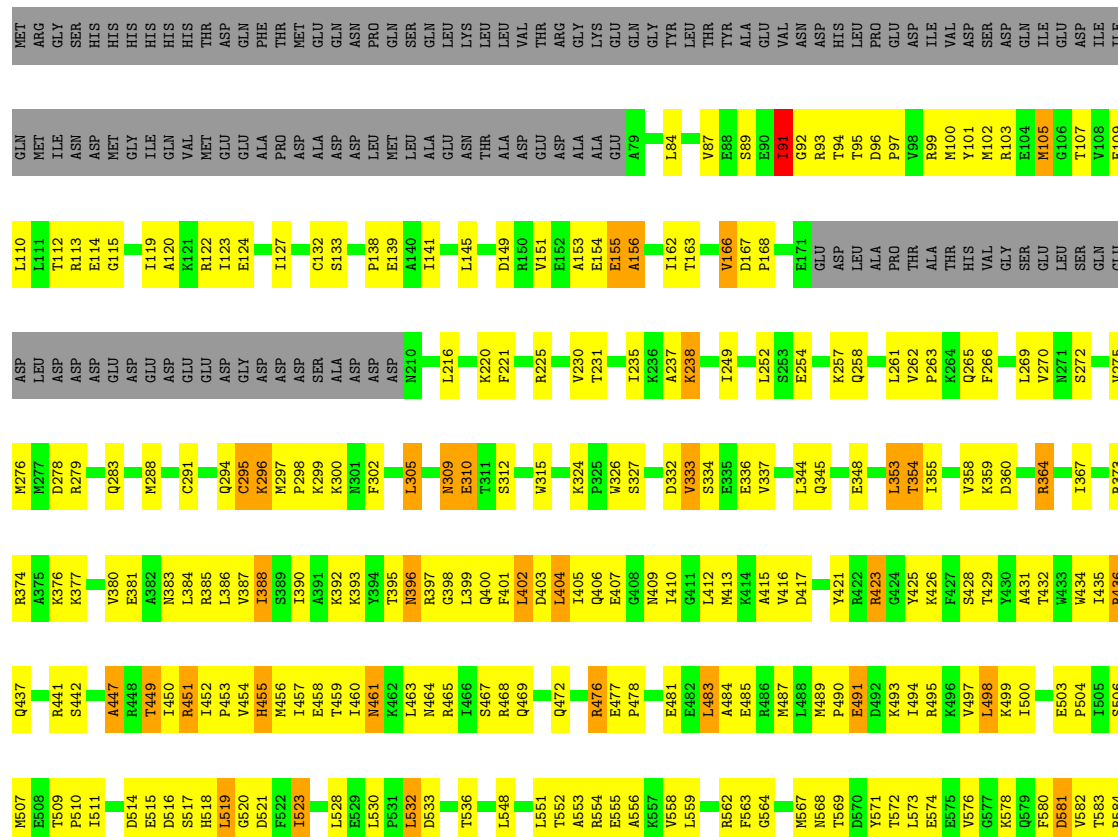
Chain F: 38% 35% 5% 21%



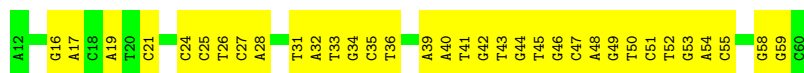


• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 37% 36% 6% 21%

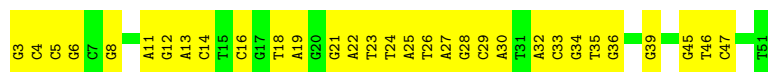


Chain 7:  31% 69%




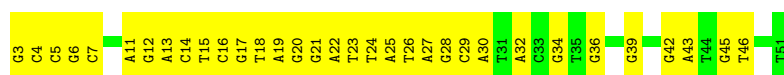
- Molecule 7: T strand DNA (49-MER)

Chain 2:  37% 63%



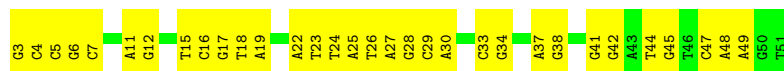
- Molecule 7: T strand DNA (49-MER)

Chain 5:  33% 67%



- Molecule 7: T strand DNA (49-MER)

Chain 8:  35% 65%



- Molecule 8: RNA (5'-D^{*}(GTP))-R(P^{*}AP^{*}GP^{*}U)-3')

Chain 3:  50% 50%



- Molecule 8: RNA (5'-D^{*}(GTP))-R(P^{*}AP^{*}GP^{*}U)-3')

Chain 6:  50% 50%



- Molecule 8: RNA (5'-D^{*}(GTP))-R(P^{*}AP^{*}GP^{*}U)-3')

Chain 9:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	240.89Å 208.17Å 256.32Å 90.00° 119.31° 90.00°	Depositor
Resolution (Å)	39.95 – 6.00 39.95 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.95-6.00) 99.6 (39.95-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 6.13Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.227 , 0.314 0.227 , 0.314	Depositor DCC
R_{free} test set	2938 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å ²)	343.5	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 229.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	94608	wwPDB-VP
Average B, all atoms (Å ²)	238.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/1809	0.85	2/2450 (0.1%)
1	B	0.57	0/1789	0.84	1/2425 (0.0%)
1	G	0.60	1/1809 (0.1%)	0.83	1/2450 (0.0%)
1	H	0.57	0/1789	0.79	1/2425 (0.0%)
1	M	0.63	0/1809	0.87	2/2450 (0.1%)
1	N	0.60	0/1789	0.87	0/2425
2	C	0.58	3/10745 (0.0%)	0.79	11/14499 (0.1%)
2	I	0.61	3/10745 (0.0%)	0.81	3/14499 (0.0%)
2	O	0.61	4/10745 (0.0%)	0.81	4/14499 (0.0%)
3	D	0.66	3/10729 (0.0%)	0.91	20/14487 (0.1%)
3	J	0.63	2/10729 (0.0%)	0.85	15/14487 (0.1%)
3	P	0.59	4/10729 (0.0%)	0.80	9/14487 (0.1%)
4	E	0.62	0/710	0.89	1/956 (0.1%)
4	K	0.56	0/710	0.72	0/956
4	Q	0.55	0/710	0.74	1/956 (0.1%)
5	F	0.56	2/4076 (0.0%)	0.77	1/5482 (0.0%)
5	L	0.59	0/4076	0.78	2/5482 (0.0%)
5	R	0.55	0/4076	0.77	2/5482 (0.0%)
6	1	0.39	0/1112	0.67	0/1706
6	4	0.51	1/1114 (0.1%)	0.73	0/1714
6	7	0.39	0/1115	0.70	0/1718
7	2	0.38	0/1136	0.66	0/1752
7	5	0.41	0/1137	0.69	0/1756
7	8	0.36	0/1137	0.68	0/1756
8	3	0.33	0/72	0.58	0/110
8	6	0.50	0/72	0.71	0/110
8	9	0.50	0/72	0.65	0/110
All	All	0.59	23/96541 (0.0%)	0.81	76/131629 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
3	P	0	1
All	All	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	316	GLU	CD-OE2	13.14	1.40	1.25
3	J	943	ARG	CZ-NH1	11.93	1.48	1.33
3	D	431	ARG	CZ-NH1	11.55	1.48	1.33
2	I	565	GLU	CB-CG	10.38	1.71	1.52
3	P	1152	GLU	CD-OE2	-9.69	1.15	1.25

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	359	LYS	CG-CD-CE	-8.94	85.08	111.90
3	D	431	ARG	NE-CZ-NH2	-8.33	116.13	120.30
3	J	943	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	M	29	GLU	C-N-CD	-7.94	103.14	120.60
3	D	376	LEU	CA-CB-CG	-7.68	97.62	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	943	ARG	Sidechain
3	P	210	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1813	190	0
1	B	1767	0	1789	200	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1787	0	1813	179	0
1	H	1767	0	1789	145	0
1	M	1787	0	1813	260	0
1	N	1767	0	1789	213	0
2	C	10576	0	10591	945	0
2	I	10576	0	10591	991	0
2	O	10576	0	10591	1002	1
3	D	10568	0	10781	1353	1
3	J	10568	0	10782	1175	0
3	P	10568	0	10780	1041	1
4	E	708	0	719	65	0
4	K	708	0	719	40	0
4	Q	708	0	719	46	0
5	F	4022	0	4083	368	1
5	L	4022	0	4083	367	0
5	R	4022	0	4083	348	0
6	1	996	0	557	71	0
6	4	996	0	555	103	1
6	7	996	0	554	69	0
7	2	1012	0	554	65	0
7	5	1012	0	553	62	0
7	8	1012	0	553	66	0
8	3	97	0	44	21	0
8	6	97	0	44	6	0
8	9	97	0	44	19	0
9	C	1	0	0	0	0
9	J	1	0	0	0	0
9	P	1	0	0	0	0
10	D	2	0	0	2	0
10	J	2	0	0	2	0
10	P	2	0	0	1	0
All	All	94608	0	92786	8368	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

The worst 5 of 8368 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:359:LYS:NZ	5:F:359:LYS:CE	1.67	1.54
3:D:484:MET:CE	3:D:484:MET:SD	2.03	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:LEU:CD2	3:P:185:ILE:HD11	1.49	1.43
3:J:367:GLY:O	3:J:447:ILE:CG2	1.68	1.38
1:G:25:LYS:NZ	1:G:202:VAL:HG11	1.34	1.37

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:12:DA:O5'	6:4:60:DC:O5'[2_454]	1.86	0.34
5:F:482:GLU:OE2	2:O:275:ARG:NH2[2_455]	1.99	0.21
3:D:1282:TYR:OH	3:P:710:ASP:OD2[1_655]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/242 (94%)	210 (92%)	15 (7%)	3 (1%)	10	42
1	B	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	4	25
1	G	228/242 (94%)	211 (92%)	14 (6%)	3 (1%)	10	42
1	H	226/242 (93%)	207 (92%)	17 (8%)	2 (1%)	14	51
1	M	228/242 (94%)	209 (92%)	16 (7%)	3 (1%)	10	42
1	N	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	5	29
2	C	1339/1342 (100%)	1218 (91%)	98 (7%)	23 (2%)	7	36
2	I	1339/1342 (100%)	1210 (90%)	102 (8%)	27 (2%)	6	31
2	O	1339/1342 (100%)	1222 (91%)	87 (6%)	30 (2%)	5	29
3	D	1360/1407 (97%)	1210 (89%)	122 (9%)	28 (2%)	5	30
3	J	1360/1407 (97%)	1225 (90%)	110 (8%)	25 (2%)	7	34
3	P	1360/1407 (97%)	1208 (89%)	112 (8%)	40 (3%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	12	47
4	K	88/90 (98%)	83 (94%)	4 (4%)	1 (1%)	12	47
4	Q	88/90 (98%)	81 (92%)	6 (7%)	1 (1%)	12	47
5	F	493/628 (78%)	443 (90%)	34 (7%)	16 (3%)	3	21
5	L	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	3	21
5	R	493/628 (78%)	441 (90%)	36 (7%)	16 (3%)	3	21
All	All	11202/11853 (94%)	10115 (90%)	841 (8%)	246 (2%)	5	29

5 of 246 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	GLY
1	A	210	THR
2	C	113	THR
2	C	481	LEU
2	C	791	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/208 (95%)	171 (86%)	27 (14%)	3	13
1	B	196/208 (94%)	172 (88%)	24 (12%)	4	15
1	G	198/208 (95%)	169 (85%)	29 (15%)	2	12
1	H	196/208 (94%)	171 (87%)	25 (13%)	3	14
1	M	198/208 (95%)	171 (86%)	27 (14%)	3	13
1	N	196/208 (94%)	167 (85%)	29 (15%)	2	12
2	C	1156/1157 (100%)	1016 (88%)	140 (12%)	4	16
2	I	1156/1157 (100%)	1013 (88%)	143 (12%)	4	15
2	O	1156/1157 (100%)	1019 (88%)	137 (12%)	4	16
3	D	1135/1168 (97%)	968 (85%)	167 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	1135/1168 (97%)	986 (87%)	149 (13%)	3	14
3	P	1135/1168 (97%)	989 (87%)	146 (13%)	3	14
4	E	74/74 (100%)	63 (85%)	11 (15%)	2	11
4	K	74/74 (100%)	70 (95%)	4 (5%)	18	40
4	Q	74/74 (100%)	68 (92%)	6 (8%)	9	28
5	F	439/554 (79%)	388 (88%)	51 (12%)	4	16
5	L	439/554 (79%)	382 (87%)	57 (13%)	3	14
5	R	439/554 (79%)	393 (90%)	46 (10%)	5	19
All	All	9594/10107 (95%)	8376 (87%)	1218 (13%)	3	14

5 of 1218 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	437	ASN
3	P	1134	ILE
2	O	637	ARG
2	O	433	ILE
3	P	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	447	HIS
3	P	1366	HIS
2	O	766	ASN
3	P	335	GLN
5	R	455	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	3/4 (75%)	1 (33%)	1 (33%)
8	6	3/4 (75%)	1 (33%)	1 (33%)
8	9	3/4 (75%)	1 (33%)	1 (33%)
All	All	9/12 (75%)	3 (33%)	3 (33%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	15	G
8	6	15	G
8	9	15	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	3	13	GTP
8	6	13	GTP
8	9	13	GTP

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	1	3
6	4	1
7	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	51:DC	O3'	52:DT	P	3.86
1	1	51:DC	O3'	52:DT	P	3.85
1	1	46:DG	O3'	47:DC	P	3.49
1	2	12:DG	O3'	13:DA	P	2.97
1	1	36:DT	O3'	37:DA	P	2.64

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/242 (95%)	-0.90	0 100 100	162, 207, 238, 299	0
1	B	228/242 (94%)	-0.83	0 100 100	165, 211, 254, 284	0
1	G	230/242 (95%)	-0.86	0 100 100	175, 216, 259, 292	0
1	H	228/242 (94%)	-0.81	1 (0%) 89 80	200, 264, 307, 325	0
1	M	230/242 (95%)	-0.85	0 100 100	155, 186, 230, 311	0
1	N	228/242 (94%)	-0.89	0 100 100	162, 205, 248, 280	0
2	C	1341/1342 (99%)	-0.93	0 100 100	126, 243, 333, 427	0
2	I	1341/1342 (99%)	-0.89	2 (0%) 92 88	142, 196, 276, 345	0
2	O	1341/1342 (99%)	-0.89	1 (0%) 92 88	126, 202, 287, 327	0
3	D	1362/1407 (96%)	-0.89	2 (0%) 92 88	129, 204, 384, 437	0
3	J	1362/1407 (96%)	-0.82	1 (0%) 92 88	145, 213, 344, 397	0
3	P	1362/1407 (96%)	-0.92	2 (0%) 92 88	133, 223, 391, 441	0
4	E	90/90 (100%)	-0.85	0 100 100	138, 184, 398, 452	0
4	K	90/90 (100%)	-0.88	0 100 100	165, 213, 389, 436	0
4	Q	90/90 (100%)	-0.97	0 100 100	157, 202, 400, 463	0
5	F	497/628 (79%)	-0.82	1 (0%) 92 85	176, 304, 513, 589	0
5	L	497/628 (79%)	-0.86	0 100 100	171, 277, 369, 399	0
5	R	497/628 (79%)	-0.85	0 100 100	170, 322, 414, 449	0
6	1	49/49 (100%)	-0.60	0 100 100	206, 263, 311, 333	0
6	4	49/49 (100%)	-0.54	0 100 100	50, 261, 289, 312	0
6	7	49/49 (100%)	-0.55	0 100 100	214, 295, 334, 336	0
7	2	49/49 (100%)	-0.58	0 100 100	183, 272, 334, 388	0
7	5	49/49 (100%)	-0.54	0 100 100	172, 257, 298, 371	0
7	8	49/49 (100%)	-0.49	0 100 100	228, 300, 347, 427	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
8	3	3/4 (75%)	-0.96	0 100 100	310, 310, 316, 331	0
8	6	3/4 (75%)	-1.01	0 100 100	242, 242, 251, 272	0
8	9	3/4 (75%)	-0.67	0 100 100	257, 257, 296, 373	0
All	All	11547/12159 (94%)	-0.87	10 (0%) 92 88	50, 219, 383, 589	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1145	PHE	4.2
3	J	1145	PHE	3.2
3	P	285	LEU	2.7
2	O	492	MET	2.7
1	H	131	CYS	2.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MG	C	1401	1/1	0.97	0.14	218,218,218,218	0
10	ZN	J	1501	1/1	0.97	0.04	218,218,218,218	0
10	ZN	D	1501	1/1	0.98	0.04	215,215,215,215	0
9	MG	J	1503	1/1	1.00	0.02	204,204,204,204	0
10	ZN	D	1502	1/1	1.00	0.05	172,172,172,172	0
9	MG	P	1503	1/1	1.00	0.01	187,187,187,187	0
10	ZN	J	1502	1/1	1.00	0.02	196,196,196,196	0
10	ZN	P	1501	1/1	1.00	0.01	252,252,252,252	0
10	ZN	P	1502	1/1	1.00	0.01	204,204,204,204	0

6.5 Other polymers [i](#)

There are no such residues in this entry.